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Applications of Matrix Calculus in the Study of Chemical Reactions

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Abstract
Linear algebra is one of the branches of algebra that has many applications in all fields of exact and technical sciences. We emphasize that one of the important applications of linear algebra is to write correctly the chemical reactions using notions of matrix calculus. Balancing chemical equations is considered the most common problem facing researchers in chemical engineering. The article contains theoretical elements that are followed by the study of five chemical reactions, which can be balanced using the Gauss-Jordan algorithm to solve a system of linear equations. The mathematical method given here is applicable to all possibility's cases in balancing chemical equations. The importance of this method lies in the fact that it becomes practically an algorithm that practically ensures the success of balancing for students who have no affinity for chemistry.

Keywords: Matrix, Gauss-Jordan algorithm, Chemical reactions.

1. Introduction
Linear algebra has long been one of the fundamental tools for mathematical disciplines with applicability in chemical engineering. It provides working methods for geometry, mathematical analysis, differential equations and especially in the study of chemical reactions [1].
Chemical reactions can be considered mathematical models. We know that any mathematical model is governed by specific rules and principles, in particular the law of conservation of mass. Using this law, we will consider chemical reactions as a system of linear equations and thus we will be able to use the Gauss-Jordan solving algorithm. In an algebraically balanced equation, the coefficients show us the number of molecules of each chemical element involved. Usually, chemical equations can be used to better understand how many products are produced from reaction given the number of reactants available [2].
The elemental reaction is the reaction in which no intermediate reaction is present. Such reactions take place in a single step. The term molecularity, applied only in elementary reactions, refers to the number of elementary particles involved in the microscopic chemical event. The representation of a chemical reaction using chemical symbols and formulas is called the chemical reaction equation [3]. The chemical equations have a double meaning: qualitative (indicates the nature of the substances and that of the reaction products. To use a chemical equation correctly, it is necessary so that it is properly balanced. If the ratio between the components of the reaction is inaccurate then the products resulting from these reactions cannot be correctly approximated which is not viable in scientific investigations. From teaching experience, I have noticed that this method has helped to balance some chemical reactions that have traditionally been considered difficult for many students [4].

2. Materials and methods
Linear algebra has many applications in various fields of science. In all technical faculties, the discipline of Linear Algebra is mandatory. In this chapter we will present the general notions of Linear Algebra that are applicable for balancing chemical reaction equations.

A linear equation in n variable is shape: $a_1x_1 + a_2x_2 + \Lambda + a_nx_n = b$, (1)

where the coefficients: $a_1, a_2, \mathrm{K}, a_n, b$ are real numbers, usually known.

In this article, we will be interested in studying the meeting of several linear equations. The meeting of these linear equations is called the system of linear equations [5].

A *system* of n equations with n unknown can be written in the form:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots\ldots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots\ldots + a_{2n}x_n = b_2 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ a_{n1}x_1 + a_{n2}x_2 + \ldots\ldots a_{nn}x_n = b_n \end{cases} \quad (2)$$

where $a_{ij}, b_i,\ i = 1,2,\mathrm{K}, n,\ j = 1,\mathrm{K}\ n,$ are constant.

Example 1:

If we consider the system: $$\begin{cases} x_1 - 2x_2 + x_3 = 5 \\ 3x_1 + 4x_2 - 7x_3 = -1 \\ 2x_1 - x_2 + 7x_3 = -9 \\ x_1 - 8x_3 = -3 \end{cases} \quad (3)$$

Then:

-The system matrix is shaped: $$A = \begin{pmatrix} 1 & -2 & 1 \\ 3 & 4 & -7 \\ 2 & -1 & 7 \\ 1 & 0 & -8 \end{pmatrix} \quad (4)$$

-The *extended* matrix is: $$\bar{A} = \begin{pmatrix} 1 & -2 & 1 & 5 \\ 3 & 4 & -7 & -1 \\ 2 & -1 & 7 & -9 \\ 1 & 0 & -8 & -3 \end{pmatrix} \quad (5)$$

Matrix of coefficients: $$b = \begin{pmatrix} 5 \\ -1 \\ -9 \\ -3 \end{pmatrix} \quad (6)$$

Definition 1: A *homogeneous* system of m equations with n unknown *can be written* as:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots\ldots + a_{1n}x_n = 0 \\ a_{21}x_1 + a_{22}x_2 + \ldots\ldots + a_{2n}x_n = 0 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ a_{m1}x_1 + a_{m2}x_2 + \ldots\ldots a_{mn}x_n = 0 \end{cases} \quad (7)$$

where $a_{ij},\ i = 1,2,\mathrm{K}, m,\ j = 1,\mathrm{K}\ n,$ are constant.

Remark 1 :

- The system (1) always supports the null solution: $x_i = 0, i = \overline{1,n}$.
- If $m = n,$ the system admits the null solution if the determinant of the associated matrix is nonzero.
- If $m = n,$ the system also admits solutions other than the null solution if the determinant of the associated matrix is zero.

Whether $A \in M_{m\times n}(R)$. *The Gauss-Jordan algorithm* for a system of homogeneous linear equations consists of the following steps[6,7] :

We will write the system matrix as well as the extended matrix.

- We will try to transform the coefficient matrix into columns of the unit matrix I_m with the help of elementary transformations.
- Variables that contain columns of the unit matrix will be called main.
- Variables that do not contain columns of the unit matrix will be called secondary and we will write them in Greek letters or sometimes we will equal them with zero.
- It is up to the reader to choose the main and secondary variables.
- We will find the solution of the system, writing the main variables according to the secondary ones [8].

3. Results & Discussion

Aluminum oxide (also called alumina) is an inorganic compound with a chemical formula Al_2O_3. It is generally used in the production of aluminum. Al_2O_3 is important for the production of metallic aluminum as an abrasive due to its hardness Aluminum oxide and carbon react to create elemental aluminum and carbon dioxide. To balance a chemical equation, a chemist must determine integers x_1, x_2, x_3, x_4 so that the total number of atoms on the left side of the chemical reaction is equal to the total number of atoms on the right side.
The chemical reaction is in shape:

$$(x_1)Al_2O_3 + (x_2)C \to (x_3)Al + (x_4)CO_2 \qquad (8)$$

Mole *distribution* in the chemical reaction: $Al_2O_3:\begin{pmatrix}2\\3\\0\end{pmatrix}, C:\begin{pmatrix}0\\0\\1\end{pmatrix}, Al:\begin{pmatrix}1\\0\\0\end{pmatrix}, CO_2:\begin{pmatrix}0\\2\\1\end{pmatrix}$, where : $\begin{pmatrix}x \to Al\\ y \to C\\ z \to O\end{pmatrix}$

To balance the chemical reaction (1), the coefficients x_1, x_2, x_3, x_4 check the system:

$$x_1\begin{pmatrix}2\\3\\0\end{pmatrix} + x_2\begin{pmatrix}0\\0\\1\end{pmatrix} = x_3\begin{pmatrix}1\\0\\0\end{pmatrix} + x_4\begin{pmatrix}0\\2\\1\end{pmatrix} \leftrightarrow \begin{cases}2x_1 - x_3 = 0\\ 3x_1 - 2x_4 = 0 \to S = \{(\alpha, \frac{3}{2}\alpha, 2\alpha, \frac{3}{2}\alpha), \alpha \in R\}\\ x_2 - x_4 = 0\end{cases}$$

$$\left(\begin{array}{cccc|c}2 & 0 & -1 & 0 & 0\\ 3 & 0 & 0 & -2 & 0\\ 0 & 1 & 0 & -1 & 0\end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c}-2 & 0 & 1 & 0 & 0\\ 3 & 0 & 0 & -2 & 0\\ 0 & 1 & 0 & -1 & 0\end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c}-2 & 0 & 1 & 0 & 0\\ -3/2 & 0 & 0 & 1 & 0\\ 0 & 1 & 0 & -1 & 0\end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c}-2 & 0 & 1 & 0 & 0\\ -3/2 & 0 & 0 & 1 & 0\\ -3.2 & 1 & 0 & 0 & 0\end{array}\right)$$

For $\alpha = 2 \to$ the balanced chemical reaction is: $2Al_2O_3 + 3C \to 4Al + 3CO_2$. (9)

Boron sulfide reacts violently with water to form boric acid and hydrogen sulfide. Considered a toxic gas with lethal potential, hydrogen sulfide has well-defined roles in the human body. Used properly, it can treat cardiovascular disease. At 500 ppm it affects our lung capacity and suffocates us, and exposure for five minutes at a concentration of 800 ppm leads to death. However, we need a small amount of hydrogen sulfide to survive. The unbalanced chemical reaction is:

$$(x_1)B_2S_3 + (x_2)H_2O \to (x_3)H_3BO_3 + (x_4)H_2S \qquad (10)$$

Mole *distribution* in the chemical reaction (2):

$$B_2S_3:\begin{pmatrix}0\\2\\0\\3\end{pmatrix}, H_2O:\begin{pmatrix}2\\0\\1\\0\end{pmatrix}, H_3BO_3:\begin{pmatrix}3\\1\\3\\0\end{pmatrix}, H_2S:\begin{pmatrix}2\\0\\0\\1\end{pmatrix}, \text{ where : } \begin{pmatrix}x \to H\\ y \to B\\ z \to O\\ t \to S\end{pmatrix}$$

To balance the chemical reaction (2), the coefficients x_1, x_2, x_3, x_4 *check the* system:

$$x_1\begin{pmatrix}0\\2\\0\\3\end{pmatrix} + x_2\begin{pmatrix}2\\0\\1\\0\end{pmatrix} = x_3\begin{pmatrix}3\\1\\3\\0\end{pmatrix} + x_4\begin{pmatrix}2\\0\\0\\1\end{pmatrix} \to \begin{cases}2x_2 - 3x_3 - 2x_4 = 0\\ 2x_1 - x_3 = 0\\ x_2 - 3x_3 = 0\\ 3x_1 - x_4 = 0\end{cases} \to S = \{(\alpha, 6\alpha, 2\alpha, 3\alpha), \alpha \in R\}$$

$$\left(\begin{array}{cccc|c} 0 & 2 & -3 & -2 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 0 & 1 & -3 & 0 & 0 \\ 3 & 0 & 0 & -1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c} 0 & 0 & 3 & -2 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 0 & 1 & -3 & 0 & 0 \\ 3 & 0 & 0 & -1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c} 0 & 0 & 3 & -2 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 0 & 1 & -3 & 0 & 0 \\ -3 & 0 & 0 & 1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c} -6 & 0 & 3 & 0 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 0 & 1 & -3 & 0 & 0 \\ -3 & 0 & 0 & 1 & 0 \end{array}\right) \leftrightarrow$$

$$\left(\begin{array}{cccc|c} -6 & 0 & 3 & 0 & 0 \\ -2 & 0 & 1 & 0 & 0 \\ 0 & 1 & -3 & 0 & 0 \\ -3 & 0 & 0 & 1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c} -6 & 0 & 3 & 0 & 0 \\ -2 & 0 & 1 & 0 & 0 \\ -6 & 1 & 0 & 0 & 0 \\ -3 & 0 & 0 & 1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{cccc|c} 0 & 0 & 0 & 0 & 0 \\ -2 & 0 & 1 & 0 & 0 \\ -6 & 1 & 0 & 0 & 0 \\ -3 & 0 & 0 & 1 & 0 \end{array}\right)$$

For $\alpha = 1 \rightarrow$ The *balanced* chemical reaction is: $B_2S_3 + 6H_2O \rightarrow 2H_3BO_3 + 3H_2S$ (11)

Calcium carbonate is the salt of calcium and carbonic acid, being a white solid with a chemical formula. $CaCO_3$. Calcium carbonate is spread in nature in the form of minerals: calcite, aragonite, water and in organisms in bones, teeth, shells, corals and crustaceans. It is estimated that about 4% of the Earth's crust is composed of calcium carbonate. The oldest structure in the world, the pyramid, is made of calcium carbonate. Calcium carbonate is recognized for its anti-acidity properties. We will consider the reaction in which calcium carbonate neutralizes acid (H_3O) so:

(3) $(x_1)H_3O + (x_2)CaCO_3 \rightarrow (x_3)H_2O + (x_4)Ca + (x_5)CO_2$ (12)

Mole distribution in the reaction **:** $H_3O : \begin{pmatrix} 0 \\ 0 \\ 3 \\ 1 \end{pmatrix}, CaCO_3 : \begin{pmatrix} 1 \\ 1 \\ 0 \\ 3 \end{pmatrix}, H_2O : \begin{pmatrix} 0 \\ 0 \\ 2 \\ 1 \end{pmatrix}, Ca : \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, CO_2 : \begin{pmatrix} 0 \\ 1 \\ 2 \\ 0 \end{pmatrix}$ To *balance* the chemical reaction (3), the coefficients x_1, x_2, x_3, x_4, x_5 *check* the system:

$$x_1\begin{pmatrix} 0 \\ 0 \\ 3 \\ 1 \end{pmatrix} + x_2\begin{pmatrix} 1 \\ 1 \\ 0 \\ 3 \end{pmatrix} = x_3\begin{pmatrix} 0 \\ 0 \\ 2 \\ 1 \end{pmatrix} + x_4\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + x_5\begin{pmatrix} 0 \\ 1 \\ 2 \\ 0 \end{pmatrix} \rightarrow \begin{cases} x_2 - x_4 = 0 \\ x_2 - x_5 = 0 \\ 3x_1 - 2x_3 - 2x_5 = 0 \\ x_1 + 3x_2 - x_3 = 0 \end{cases}$$

$$\left(\begin{array}{ccccc|c} 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 3 & 0 & -2 & 0 & -2 & 0 \\ 1 & 3 & -1 & 0 & 0 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 3 & 0 & -2 & 0 & -2 & 0 \\ 1 & 3 & -1 & 0 & 0 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 3 & 0 & -2 & 0 & -2 & 0 \\ 1 & 3 & -1 & 0 & 0 & 0 \end{array}\right) \leftrightarrow$$

$$\left(\begin{array}{ccccc|c} 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 3 & 0 & -2 & 0 & -2 & 0 \\ 1 & 0 & -1 & 0 & 3 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & -2/3 & 0 & -2/3 & 0 \\ 1 & 0 & -1 & 0 & 3 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & -2/3 & 0 & -2/3 & 0 \\ 0 & 0 & -1/3 & 0 & 11/3 & 0 \end{array}\right) \leftrightarrow$$

$$\left(\begin{array}{ccccc|c} 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & -2/3 & 0 & -2/3 & 0 \\ 0 & 0 & 1 & 0 & -11 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & -8 & 0 \\ 0 & 0 & 1 & 0 & -11 & 0 \end{array}\right) \leftrightarrow S = \{(8\alpha, \alpha, 11\alpha, \alpha, \alpha), \alpha \in R\}$$

For $\alpha = 1$,the *balanced* chemical reaction is: $8H_3O + CaCO_3 \rightarrow 11H_2O + Ca + CO_2$ (13)

Alka-Seltzer is an effervescent antacid and analgesic and contains three active ingredients: aspirin (acetylsalicylic acid) (ASA), baking soda and anhydrous citric acid. It is used to combat pain of low or moderate intensity, in headaches, myalgia, rheumatic joint and periarticular pain, neuralgia, dental pain, dysmenorrhea, fighting fever. As an inflammatory it can be used to combat inflammatory phenomena in acute polyarticular rheumatism; attenuation of joint inflammation in rheumatoid arthritis. Alka-Seltzer should not be used for more than 3-5 days without consulting your doctor. Alka-Seltzer contains baking soda ($NaHCO_3$) and citric acid ($H_3C_6H_5O_7$). When the tablet is dissolved in water, the reaction takes place:

$$(x_1)NaHCO_3 + (x_2)H_3C_6H_5O_7 \to (x_3)Na_3C_6H_5O_7 + (x_4)H_2O + (x_5)CO_2 \tag{14}$$

Mole distribution in the reaction (4):

$$NaHCO_3 : \begin{pmatrix}1\\1\\1\\3\end{pmatrix}, H_3C_6H_5O_7 : \begin{pmatrix}0\\8\\6\\7\end{pmatrix}, Na_3C_6H_5O_7 : \begin{pmatrix}3\\5\\6\\7\end{pmatrix}, H_2O : \begin{pmatrix}0\\2\\0\\1\end{pmatrix}, CO_2 : \begin{pmatrix}0\\0\\1\\2\end{pmatrix}$$

To balance the chemical reaction (4), the coefficients x_1, x_2, x_3, x_4, x_5 *check* the system:

$$x_1\begin{pmatrix}1\\1\\1\\3\end{pmatrix} + x_2\begin{pmatrix}0\\8\\6\\7\end{pmatrix} = x_3\begin{pmatrix}3\\5\\6\\7\end{pmatrix} + x_4\begin{pmatrix}0\\2\\0\\1\end{pmatrix} + x_5\begin{pmatrix}0\\0\\1\\1\end{pmatrix} \to \begin{cases} x_1 - 3x_3 = 0 \\ x_1 + 8x_2 - 5x_3 - 2x_4 = 0 \\ x_1 + 6x_2 - 6x_3 - x_5 = 0 \\ 3x_1 + 7x_2 - 7x_3 - x_4 - x_5 = 0 \end{cases}$$

$$\left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 1 & 8 & -5 & -2 & 0 & 0 \\ 1 & 6 & -6 & 0 & -1 & 0 \\ 3 & 7 & -7 & -1 & -1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 8 & -2 & -2 & 0 & 0 \\ 1 & 6 & -6 & 0 & -1 & 0 \\ 3 & 7 & -7 & -1 & -1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 8 & -2 & -2 & 0 & 0 \\ 0 & 6 & -3 & 0 & -1 & 0 \\ 3 & 7 & -7 & -1 & -1 & 0 \end{array}\right) \leftrightarrow$$

$$\left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 8 & -2 & -2 & 0 & 0 \\ 0 & 6 & -3 & 0 & -1 & 0 \\ 0 & 7 & 2 & -1 & -1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 8 & -2 & -2 & 0 & 0 \\ 0 & 6 & -3 & 0 & -1 & 0 \\ 0 & -7 & -2 & 1 & 1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & -6 & -6 & 0 & 2 & 0 \\ 0 & 6 & -3 & 0 & -1 & 0 \\ 0 & -7 & -2 & 1 & 1 & 0 \end{array}\right) \leftrightarrow$$

$$\left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & -6 & -6 & 0 & 2 & 0 \\ 0 & -6 & 3 & 0 & 1 & 0 \\ 0 & -7 & -2 & 1 & 1 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & -6 & -6 & 0 & 2 & 0 \\ 0 & -6 & 3 & 0 & 1 & 0 \\ 0 & -1 & -5 & 1 & 0 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 6 & -12 & 0 & 0 & 0 \\ 0 & -6 & 3 & 0 & 1 & 0 \\ 0 & -1 & -5 & 1 & 0 & 0 \end{array}\right) \leftrightarrow$$

$$\left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 \\ 0 & -6 & 3 & 0 & 1 & 0 \\ 0 & -1 & -5 & 1 & 0 & 0 \end{array}\right) \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & -9 & 0 & 1 & 0 \\ 0 & -1 & -5 & 1 & 0 & 0 \end{array}\right) \leftrightarrow \left(\begin{array}{ccccc|c} 1 & 0 & -3 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & -9 & 0 & 1 & 0 \\ 0 & 0 & -7 & 1 & 0 & 0 \end{array}\right) \leftrightarrow S = \{(3\alpha, 2\alpha, \alpha, 7\alpha, 9\alpha), \alpha \in R\}$$

For $\alpha = 1 \to$ The balanced reaction is: $3NaHCO_3 + 2H_3C_6H_5O_7 \to Na_3C_6H_5O_7 + 7H_2O + 9CO_2$ (15)

Lead minium, also called lead red or Saturn red, is a synthetic pigment, a bright red-orange lead oxide. It is not resistant to concentrated acids and bases and is not stable to light and air. Minimum Lead Mixture (Pb_3O_4). Aluminum powder was in vogue in the 1980s when it was very easy to obtain commercially. Firecrackers with that mixture make a very deep and extremely loud noise, they are very simple to make. Due to its toxicity, it is no longer used in painting. We will try to balance this reaction of producing lead mini.

Either the reaction from which lead minium is obtained:.

$$(x_1)PbN_6 + (x_2)CrMn_2O_8 \to (x_3)Pb_3O_4 + (x_4)Cr_2O_3 + (x_5)MnO_2 + (x_6)NO \tag{16}$$

Mole distribution in the reaction (5):

$$PbN_6 : \begin{pmatrix}1\\6\\0\\0\\0\end{pmatrix}, CrMn_2O_8 : \begin{pmatrix}0\\0\\1\\2\\8\end{pmatrix}, Pb_3O_4 : \begin{pmatrix}3\\0\\0\\0\\4\end{pmatrix}, Cr_2O_3 : \begin{pmatrix}0\\0\\2\\0\\3\end{pmatrix}, MnO_2 : \begin{pmatrix}0\\0\\0\\1\\2\end{pmatrix}, NO : \begin{pmatrix}0\\1\\0\\0\\1\end{pmatrix}$$

To *balance* the chemical reaction (4), the coefficients $x_1, x_2, x_3, x_4, x_5, x_6$ check the system:

$$x_1\begin{pmatrix}1\\6\\0\\0\\0\end{pmatrix}+x_2\begin{pmatrix}0\\0\\1\\2\\8\end{pmatrix}=x_3\begin{pmatrix}3\\0\\0\\0\\4\end{pmatrix}+x_4\begin{pmatrix}0\\0\\2\\0\\3\end{pmatrix}+x_5\begin{pmatrix}0\\0\\0\\1\\2\end{pmatrix}+x_6\begin{pmatrix}0\\1\\0\\0\\1\end{pmatrix}\leftrightarrow\begin{cases}x_1-3x_3=0\\6x_1-x_6=0\\x_2-2x_4=0\\2x_2-x_5=0\\8x_2-4x_3-3x_4-2x_5-x_6=0\end{cases}$$

$$\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\6&0&0&0&0&-1&0\\0&1&0&-2&0&0&0\\0&2&0&0&-1&0&0\\0&8&-4&-3&-2&-1&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&18&0&0&-1&0\\0&1&0&-2&0&0&0\\0&2&0&0&-1&0&0\\0&8&-4&-3&-2&-1&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&2&0&0&-1&0&0\\0&8&-4&-3&-2&-1&0\end{array}\right)\leftrightarrow$$

$$\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&2&0&0&-1&0&0\\0&8&-22&-3&-2&0&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&0&0&4&-1&0&0\\0&8&-22&-3&-2&0&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&0&0&4&-1&0&0\\0&0&-22&13&-2&0&0\end{array}\right)\leftrightarrow$$

$$\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&0&0&-4&1&0&0\\0&0&-22&13&-2&0&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&0&0&-4&1&0&0\\0&0&-22&5&0&0&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&0&0&-4&1&0&0\\0&0&-22/5&1&0&0&0\end{array}\right)\leftrightarrow$$

$$\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&0&-2&0&0&0\\0&0&-88/5&0&1&0&0\\0&0&-22/5&1&0&0&0\end{array}\right)\leftrightarrow\left(\begin{array}{cccccc|c}1&0&-3&0&0&0&0\\0&0&-18&0&0&1&0\\0&1&-44/5&0&0&0&0\\0&0&-88/5&0&1&0&0\\0&0&-22/5&1&0&0&0\end{array}\right)\leftrightarrow\begin{cases}x_1=3\alpha\\x_2=\dfrac{44}{5}\alpha\\x_3=\alpha\\x_4=\dfrac{22}{5}\alpha,\alpha\in R\\x_5=\dfrac{88}{5}\alpha\\x_6=18\alpha\end{cases}$$

For $\alpha=5\rightarrow$ The balanced reaction is: $15PbN_6+44CrMn_2O_8\rightarrow 5Pb_3O_4+22Cr_2O_3+88MnO_2+90NO$ (17)

4. Conclusions

The models represented by differential equations presented in this article offer some significant advantages compared to other models proposed in chemistry, namely: they can model evolutionary processes, allow a compartmental analysis of the modeled process, allow determining the stability of equilibrium configurations, allow sensitivity analysis ¸ in relation to the reaction parameters. From a mathematical point of view, the theory of differential equations is well developed both qualitatively and numerically. As a disadvantage, they cannot model phenomena with a high degree of heterogeneity. These models can be used successfully in developing inverse methods for determining one or more reaction parameters involved in the model. The accuracy of the predictions of these models is strongly influenced by the internal kinetics, by the spatial-temporal scale of evaluation of the reaction parameters, by the control of the error of solving the mathematical model. An extremely useful principle used in modeling chemical reactions has proven to be the principle of mass conservation.

References

1. Flowers P, Theopold K, Langley R., Robinson W. Chemistry, 7th ed., 2015.
2. Lay S. R., Judi J. M. Linear Algebra and Its Applications (5th Edition). 2015.
3. Clugston M., Flemming, R. Advanced chemistry: Oxford University Press,2002.
4. Lay D. C., Linear algebra and its applications, Pearson Education, 2006.
5. Gilbert S. Introduction to Linear Algebra (4th ed.). United Kingdom: WellesleyCambridge Press, 2009.

6. DeFranza J., Gagliardi D. Introduction to Linear Algebra with Applications. New York, McGraw-Hill,2009
7. David P. Linear Algebra: A Modern Introduction. United Kingdom, 2010.
8. Thomas S. Applied Linear Algebra and Matrix Analysis, Undergraduate Texts in Mathematics. Germany: Springer, 2006.